

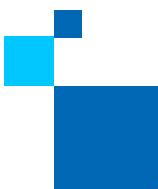
Intel® DPC++ Compatibility Tool

Migration Experiences Sharing

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intel.[®]

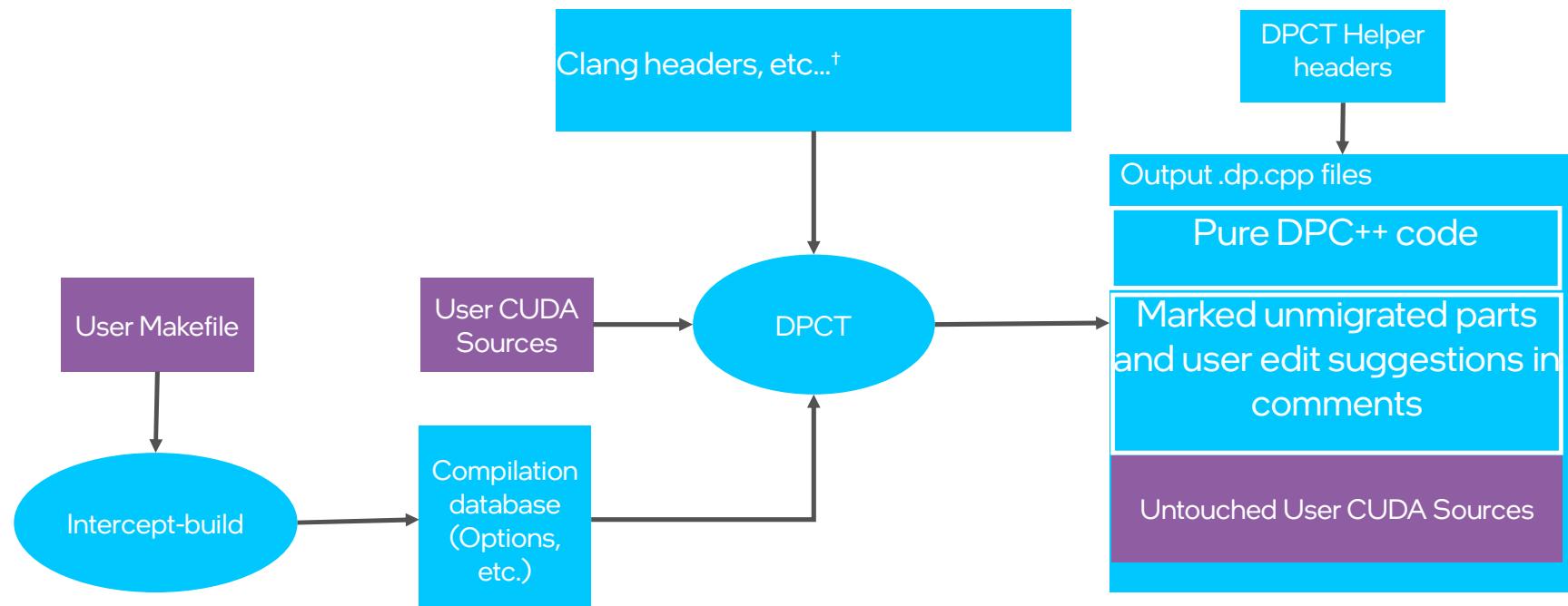
DSC

Agenda

- High-level workflow
- Common practices in large project migration
- New features to ease build & release
- Texture/image code migration
- Experimental features
- Workarounds in original CUDA project

High-level workflow

High-level Workflow



Command line example:
intercept-build make

Command line example:
cd rodinia_3.1/cuda/nw
dpct -p . --in-root=./ --out-root=dpct_output --keep-original-code needle.cu

[†] Certain CUDA header files may need to be available

DPCT Helpers

Intel > oneAPI > dpcpp-ct > 2022.0.0 > include > dpct			
Name	Date modified	Type	Size
dpl_extras	12/16/2021 5:10 PM	File folder	
atomic.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	13 KB
blas_utils.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	22 KB
device.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	15 KB
dpct.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	2 KB
dpl_utils.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	1 KB
image.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	32 KB
kernel.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	2 KB
memory.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	45 KB
util.hpp	10/31/2021 6:12 AM	UltraEdit Document (.hpp)	12 KB

- DPCT implements common code patterns to assist the migration of input source code as a set of header files.
- Uses SYCL style and oneAPI libraries, e.g., oneMKL, oneDPL

Migration of large cmake-style project

Basic Options of Intel® DPC++ Compatibility Tool

- `--in-root=<dir>`: path for the root of the source tree that needs to be migrated
- `--out-root=<dir>`: path for root of generated files (NOT specify the same with `-in-root`)
- `-p=<dir>`: path for the compilation database
- `--process-all` : Migrates or copies all files from the `--in-root` directory to the `--out-root` directory
- `--keep-original-code` : Keeps the original code in comments of generated DPC++ files
- `--extra-arg=<string>` : Specify more compiler options (The options that can be passed this way can be found with the `dpct -- -help` command.)
(Using `dpct --help` to get all the options of dpct)

Common Practices

- Know the build configuration components of the large CUDA project
 - Some configuration options are necessary to enable CUDA code base
- Get the compilation database via ‘intercept-build make target’
 - ‘target’ limits the set of CUDA files to those you are interested in.
- Run dpct pointing to compilation database and ‘–process-all’
- Use dpcpp to compile output DPC++ code
- Integrate new DPC++ code base back to the large project

Relion migration

oneAPI > relion-master > src > apps

Name
motion_refine_mpi.cpp
motion_stats.cpp
mrc2vtk.cpp
paper_data_synth.cpp
particle_polish.cpp
particle_polish_mpi.cpp
particle_reposition.cpp
particle_sort.cpp
particle_sort_mpi.cpp
particle_symmetry_expand.cpp
pipeliner.cpp
postprocess.cpp
postprocess_mpi.cpp
prepare_subtomo.cpp
preprocess.cpp
preprocess_mpi.cpp
project.cpp
reconstruct.cpp
reconstruct_mpi.cpp
ref_aberration_plot.cpp
refine.cpp
refine_mpi.cpp

Configure and running with standard benchmarks 3D classification from
https://www3.mrc-lmb.cam.ac.uk/relion/index.php/Benchmarks_%26_computer_hardware

```
'CC=icx CXX=dpcpp cmake -DCUDA_ARCH=70 -DCUDA=ON -DCudaTexture=OFF -  
DGUI=OFF -DCMAKE_BUILD_TYPE=DEBUG -DBUILD_SHARED_LIBS=OFF -D  
CMAKE_C_FLAGS="-O0 -g" -D CMAKE_CXX_FLAGS="-O0 -g" ..'  
  
bin/relion_refine: src/apps/CMakeFiles/refine.dir/refine.cpp.o  
bin/relion_refine: src/apps/CMakeFiles/refine.dir/build.make  
bin/relion_refine: lib/librelion.lib.a  
bin/relion_refine: /usr/local/cuda-10.1/lib64/libcufft.so  
bin/relion_refine: /usr/lib/x86_64-linux-gnu/openmpi/lib/libmpi_cxx.so  
bin/relion_refine: /usr/lib/x86_64-linux-gnu/openmpi/lib/libmpi.so  
bin/relion_refine: lib/librelion_gpu_util.a  
bin/relion_refine: /usr/lib/x86_64-linux-gnu/libtiff.so  
bin/relion_refine: /usr/lib/x86_64-linux-gnu/libtiff.so  
bin/relion_refine: lib/librelion.lib.a  
bin/relion_refine: lib/librelion_gpu_util.a  
bin/relion_refine: /usr/lib/x86_64-linux-gnu/libfftw3f.so  
bin/relion_refine: /usr/lib/x86_64-linux-gnu/libfftw3.so  
bin/relion_refine: /usr/local/cuda-10.1/lib64/libcurand.so  
bin/relion_refine: /usr/local/cuda-10.1/lib64/libcudart_static.a  
bin/relion_refine: /usr/lib/x86_64-linux-gnu/librt.so  
bin/relion_refine: /usr/local/cuda-10.1/lib64/libcufft.so  
bin/relion_refine: src/apps/CMakeFiles/refine.dir/link.txt
```

build\src\apps\C
MakeFiles\refine.
dir\build.make

LIBRELION_GPU_UTIL

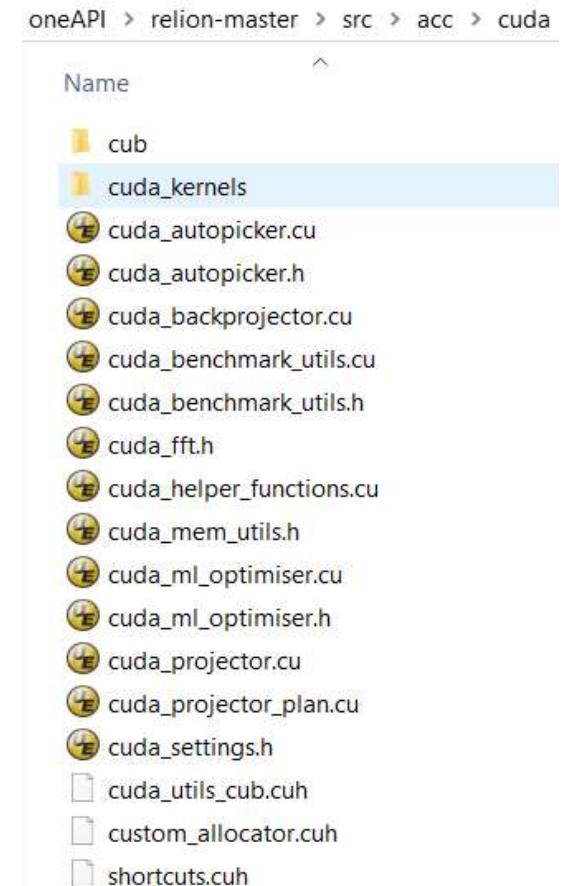
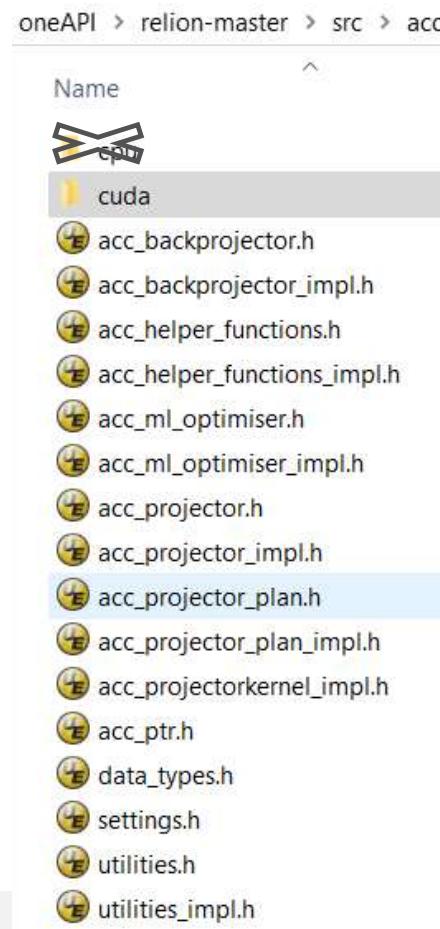
```

agent_histogram.cuh
agent_radix_sort_downsweep.cuh
agent_radix_sort_upsweep.cuh
agent_reduce.cuh
agent_reduce_if.cuh
agent_reduce_by_key.cuh
agent_rle.cuh
agent_scan.cuh
agent_segment_fixup.cuh
agent_select_if.cuh
agent_spmv_csr.cuh
agent_spmv_orig.cuh
agent_spmv_row_based.cuh
arg_index_input_iterator.cuh
block_adjacent_difference.cuh
block_discontinuity.cuh
block_exchange.cuh
block_histogram.cuh
block_histogram_atomic.cuh
block_histogram_sort.cuh
block_load.cuh
block_radix_rank.cuh
block_radix_sort.cuh
block_raking_layout.cuh
block_reduce.cuh
block_reduce_raking.cuh
block_reduce_raking_commutative_only.cuh
block_reduce_warp_reductions.cuh
block_scan.cuh
block_scan_raking.cuh
block_scan_warp_scans.cuh
block_scan_warp_scans2.cuh
block_scan_warp_scans3.cuh
block_shuffle.cuh
block_store.cuh

BP.cuh
cache_modified_input_iterator.cuh
cache_modified_output_iterator.cuh
constant_input_iterator.cuh
counting_input_iterator.cuh
cub.cuh
cuda_device_utils.cuh
cuda_utils.cuh
custom_allocator.cuh
device_histogram.cuh
device_partition.cuh
device_radix_sort.cuh
device_reduce.cuh
device_run_length_encode.cuh
device_scan.cuh
device_segmented_radix_sort.cuh
device_segmented_reduce.cuh
device_select.cuh
device_spmv.cuh
diff2.cuh
discard_output_iterator.cuh
dispatch_histogram.cuh
dispatch_radix_sort.cuh
dispatch_reduce.cuh
dispatch_reduce_by_key.cuh
dispatch_rle.cuh
dispatch_scan.cuh
dispatch_select_if.cuh
dispatch_spmv_csr.cuh
dispatch_spmv_orig.cuh
dispatch_spmv_row_based.cuh
grid_barrier.cuh
grid_even_share.cuh
grid_mapping.cuh

grid_queue.cuh
helper.cuh
mutex.cuh
shortcuts.cuh
single_pass_scan_operators.cuh
tex_obj_input_iterator.cuh
tex_ref_input_iterator.cuh
thread_load.cuh
thread_operators.cuh
thread_reduce.cuh
thread_scan.cuh
thread_search.cuh
thread_store.cuh
transform_input_iterator.cuh
util_allocator.cuh
util_arch.cuh
util_debug.cuh
util_device.cuh
util_macro.cuh
util_namespace.cuh
util_ptx.cuh
util_type.cuh
warp_reduce.cuh
warp_reduce_shfl.cuh
warp_reduce_smem.cuh
warp_scan.cuh
warp_scan_shfl.cuh
warp_scan_smem.cuh
wavg.cuh

```



Migrate and Build

- make clean
- intercept-build make relion_gpu_util
- dpct -p=./build --in-root=./ --out-root=dpct_output --keep-original-code –process-all
- Review/update manually the resulting DPC++ code.
 - Rename MACROs from original CUDA code e.g. replace 'CUDA' with 'DPCPP'
 - DPCT automatically replaces the '__CUDA_ARCH__' with 'DPCT_COMPATIBILITY_TEMP', but no more.
- dpcpp -a -O0 -c *.dp.cpp cuda_kernels/helper.dp.cpp -I[root of relion] -I[root of relion]/external/fftw/include
-DDPCPP(was -DCUDA) -DPROJECTOR_NO_TEXTURES -DHAVE_SINCOS -DHAVE_TIFF
- ar cr librelion_gpu_util.a *.o
- make refine (host part build)
- dpcpp -g -O0 -DDEBUG_CUDA -fopenmp -rdynamic
.src/apps/CMakeFiles/refine.dir/refine.cpp.o -o ./bin/relion_refine -Wl,-rpath,[root of
relion]/external/fftw/lib:./lib/librelion_lib.a -ltiff ./lib/librelion_lib.a ./lib/librelion_gpu_util.a
..../external/fftw/lib/libfftw3.so/external/fftw/lib/libfftw3f.so -lpthread -ldl -lrt

Enhancements in build and release

New Options of Intel® DPC++ Compatibility Tool 2022.0

- **--gen-build-script**
 - generates makefile for migrated file(s) in -out-root directory
- **--build-script-file=<file>**
 - name of generated makefile for migrated file(s). Default name: Makefile.dpct.
- **--use-custom-helper=<value>**
 - customize the DPCT helper header files for migrated code and place them in the --out-root directory. The values are: none, file, api, all

MAGMA project Makefile.dpct snippet via –gen-build-script

```
CC := dpcpp

LD := $(CC)

#DPCT2001:8814: You can link with more library by add them here.
LIB :=

FLAGS :=

TARGET_0_SRC_0 = ./control/abs.cpp.dp.cpp
TARGET_0_OBJ_0 = ./control/abs.cpp.dp.o
TARGET_0_FLAG_0 = -O3 -DADD_ -I./control -I ./include ${FLAGS}

.PHONY:all clean
OBJS_0 := ${TARGET_0_OBJ_0} ${TARGET_0_OBJ_1} ${TARGET_0_OBJ_2} ${TARGET_0_OBJ_3} ${TARGET_0_OBJ_4} ${TARGET_0_O
${TARGET_0_OBJ_6} ${TARGET_0_OBJ_7} ${TARGET_0_OBJ_8} ${TARGET_0_OBJ_9} ${TARGET_0_OBJ_10} ${TARGET_0_OBJ_11}
${TARGET_0_OBJ_12} ${TARGET_0_OBJ_13} ${TARGET_0_OBJ_14} ${TARGET_0_OBJ_15} ${TARGET_0_OBJ_16} ${TARGET_0_OBJ_17}
${TARGET_0_OBJ_18} ${TARGET_0_OBJ_19} ${TARGET_0_OBJ_20} ${TARGET_0_OBJ_21} ${TARGET_0_OBJ_22} ${TARGET_0_OBJ_23}

OBJS := ${OBJS_0}

all: ${OBJS}

${TARGET_0_OBJ_0}: ${TARGET_0_SRC_0}
    $(CC) -c ${TARGET_0_SRC_0} -o ${TARGET_0_OBJ_0} ${TARGET_0_FLAG_0}
```

Release with only necessary DPCT helpers

```
dpct --out-root=dpct_output CopyTex2D.cu --use-custom-helper=api
```

include > dpct

Name	Size
device.hpp	5 KB
dpct.hpp	1 KB
image.hpp	22 KB
memory.hpp	13 KB
util.hpp	1 KB

Intel > oneAPI > dpcpp-ct > 2022.0.0 > include > dpct

Name	Size
dpl_extras	
atomic.hpp	13 KB
blas_utils.hpp	22 KB
device.hpp	15 KB
dpct.hpp	2 KB
dpl_utils.hpp	1 KB
image.hpp	32 KB
kernel.hpp	2 KB
memory.hpp	45 KB
util.hpp	12 KB

Texture sample migration



SYCL image support limitation

- DPC++ RT supports 4-channel image format ONLY
- DPCT supports migration of more scenarios, than what is supported currently by SYCL
- Manual edit needed in DPCT output for both –
 - Image format
 - Input data layout

2D Texture in CUDA

```
texture<int, 2> textureD;
__global__ void kernel(int *doutput,
int width)
{
    int row = threadIdx.y;
    int col = threadIdx.x;
    doutput[row * width + col] =
tex2D(textureD, col, row);
}

int *d; size_t pitch;
cudaMallocPitch(&d, &pitch, ...);
cudaChannelFormatDesc channel =
cudaCreateChannelDesc<int>();
cudaBindTexture2D(NULL, &textureD, d,
&channel, width, height, pitch);
kernel<<<1, (width, height)>>>(doutput,
width);
```

Output from DPCT :

```
/*
```

DPCT1059:2: SYCL only supports 4-channel image format. Adjust the code.

```
*/
```

```
dpct::image_wrapper<int, 2> textureD;
```

```
/*
```

DPCT1059:3: SYCL only supports 4-channel image format. Adjust the code.

```
*/
```

```
dpct::image_channel channel =
dpct::image_channel::create<int>();
```



DPCT1059

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DPCT1004
DPCT1005
DPCT1006
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DPCT1008
DPCT1009

DPCT1059

Message

SYCL only supports 4-channel image format. Adjust the code.

Detailed Help

SYCL* supports only 4-channel image format. The warning is emitted, when the tool generates code with unsupported image format, which corresponds to the original code. You can fix the resulting code by changing the image format. Note: suggested workaround may impact code performance.

For example, the following migrated DPC++ code:

```
1 // migrated DPC++ code, which is using unsupported image format:  
2  
3 dpct::image_wrapper<cl::sycl::uint2, 2> tex; // 2-channel image is not  
4 supported  
5  
6 void test_image(dpct::image_accessor_ext<cl::sycl::uint2, 2> acc) {  
7     cl::sycl::uint2 tex_data;  
8     tex_data = acc.read(0, 0);  
9 }
```

[Refer to Compatibility Tool – Diagnostic Reference](#)

Image format adjustment

```
texture<int, 2> textureD;
__global__ void kernel(int *doutput,
int width)
{
    int row = threadIdx.y;
    int col = threadIdx.x;
    doutput[row * width + col] =
tex2D(textureD, col, row);
}
```

```
/*
DPCT1059:2: SYCL only supports 4-channel
image format. Adjust the code.
*/
dpct::image_wrapper<sycl::int4, 2> textureD;

void kernel(int *doutput, int width,
sycl::nd_item<3> item_ct1,
dpct::image_accessor_ext<sycl::int4, 2>
textureD)

{
    int row = item_ct1.get_local_id(1);
    int col = item_ct1.get_local_id(2);
    doutput[row * width + col] =
textureD.read(col, row)[0];
}
```

Input data layout adjustment

```
int *d; size_t pitch;
cudaMallocPitch(&d, &pitch, width *
sizeof(int), height);

cudaMemcpy2D(d, pitch, h, width *
sizeof(int), width * sizeof(int),
height, cudaMemcpyHostToDevice);

cudaChannelFormatDesc channel =
cudaCreateChannelDesc<int>();

cudaBindTexture2D(NULL, &textureD,
d, &channel, width, height, pitch);
```

```
int *d; size_t pitch;
d = (int *)dpct::dpct_malloc(pitch, width *
sizeof(sycl::int4), height);

dpct::dpct_memcpy(d, pitch, h, width *
sizeof(sycl::int4), width* sizeof(sycl::int4),
height, dpct::host_to_device);
/*
DPCT1059:3: SYCL only supports 4-channel
image format. Adjust the code.
*/
dpct::image_channel channel =
dpct::image_channel::create<sycl::int4>();

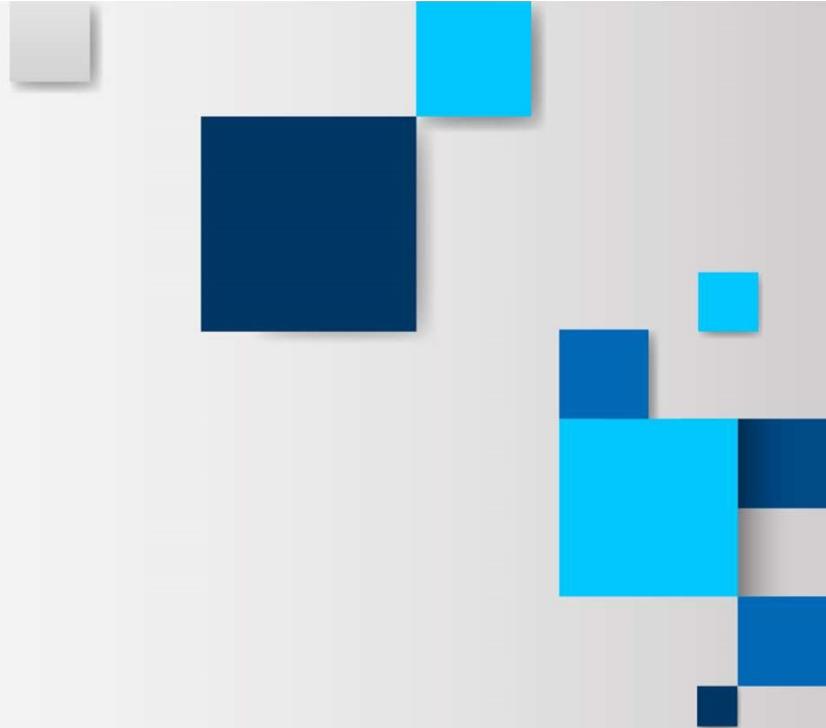
textureD.attach(d, width, height, pitch,
channel);
```

Kernel invocation

```
kernel
<<<1,(width,height)>>>
(doutput, width);
```

```
sycl::range<3> PerBlock(1, height, width);
q_ct1.submit([&](sycl::handler &cgh) {
    auto textureD_acc =
textureD.get_access(cgh);
    auto textureD_smp1 =
textureD.get_sampler();
    cgh.parallel_for(
        sycl::nd_range<3>(PerBlock, PerBlock),
        [=](sycl::nd_item<3> item_ct1) {
            kernel(doutput, width, item_ct1,
dpct::image_accessor_ext<sycl::int4,2>
(textureD_smp1, textureD_acc));
        });
});
```

Experimental features



Use experimental features of Intel® DPC++ Compatibility Tool

- **--use-experimental-features=<value>**

Comma separated list of experimental features to be used in migrated code.
By default, experimental features will not be used in migrated code.

The values are:

=nd_range_barrier

- cross group synchronization during migration.

=free-function-queries

- allows to get `id`, `item`, `nd_item`, `group`, `sub_group` instances.

Across group synchronization not available currently in SYCL

```
#include <cooperative_groups.h>
#include <cuda_runtime.h>

namespace cg = cooperative_groups;

__global__ void kernel() {
    cg::grid_group grid = cg::this_grid();
    grid.sync();

    printf("Hello\n");
}

int main() {
    kernel<<<16, 4>>>();
    cudaDeviceSynchronize();

    return 0;
}
```

```
void kernel(const sycl::stream &stream_ct1) {
/*
DPCT1087:2: DPC++ currently does not support cross group
synchronization, you
can specify "--use-experimental-
features=nd_range_barrier" to use the dpct
helper function nd_range_barrier to migrate grid.sync().
*/
    cg::grid_group grid = cg::this_grid();
/*
DPCT1087:0: DPC++ currently does not support cross group
synchronization, you
can specify "--use-experimental-
features=nd_range_barrier" to use the dpct
helper function nd_range_barrier to migrate grid.sync().
*/
    grid.sync();
}
```

--use-experimental-features=nd_range_barrier

```
void kernel(sycl::nd_item<3> item_ct1, sycl::ONEAPI::atomic_ref<unsigned int, sycl::ONEAPI::memory_order::seq_cst, sycl::ONEAPI::memory_scope::device, sycl::access::address_space::global_space> &sync_ct1) {
    dpct::experimental::nd_range_barrier(item_ct1, sync_ct1);
}

dpct::experimental::nd_range_barrier(item_ct1, sync_ct1);
}

dpct::get_default_queue().submit([&](sycl::handler &cah) {
    dpct::global_memory<unsigned int, 0> d_sync_ct1(0);
    unsigned *sync_ct1 = d_sync_ct1.get_ptr(dpct::get_default_queue());
    dpct::get_default_queue().memset(sync_ct1, 0, sizeof(int)).wait();

    cgh.parallel_for(sycl::nd_range<3>(...), [=](sycl::nd_item<3> item_ct1) {
        auto atm_sync_ct1 = sycl::ONEAPI::atomic_ref<unsigned int, ...seq_cst,
            ...memory_scope::device,...address_space::global_space>(sync_ct1[0]);
        kernel(item_ct1, atm_sync_ct1);
    });
});
dpct::get_current_device().queues_wait_and_throw();
```

Functor migration – default behavior

```
struct SplitNodes
{
    int maxPointsPerNode;
    int* node_count;
    int* nodes_allocated;
    int* out_of_space;
    int* child1_;
    int* parent_;
    SplitInfo* splits;

    __device__
    void operator()( thrust::tuple<int&, int&, SplitInfo&, float4&, float4&, int> node )
    {
        int& parent=thrust::get<0>(node);
        int& child1=thrust::get<1>(node);
        SplitInfo& s=thrust::get<2>(node);
        const float4& aabbMin=thrust::get<3>(node);
        const float4& aabbMax=thrust::get<4>(node);
        int my_index = thrust::get<5>(node);
        bool split_node=false;
        // first, each thread block counts the number of nodes that it needs to allocate
        __shared__ int block_nodes_to_allocate;
        if( threadIdx.x== 0 ) block_nodes_to_allocate=0;
        __syncthreads();
    }
}
```

Code snippet from - https://github.com/flann-lib/flann/blob/master/src/cpp/flann/algorithms/kdtree_cuda_builder.h

```
struct SplitNodes
{
    int maxPointsPerNode;
    int* node_count;
    int* nodes_allocated;
    int* out_of_space;
    int* child1_;
    int* parent_;
    SplitInfo* splits;

    void operator()(std::tuple<int &, int &, SplitInfo &, sycl::float4 &, sycl::float4 &, int>
                     node,
                     sycl::nd_item<3> item_ctl, int *block_nodes_to_allocate,
                     int *block_left,
                     bool *enough_space) // float4: aabbMin, aabbMax
    {
        int &parent = std::get<0>(node);
        int &child1 = std::get<1>(node);
        SplitInfo &s = std::get<2>(node);
        const sycl::float4 &aabbMin = std::get<3>(node);
        const sycl::float4 &aabbMax = std::get<4>(node);
        int my_index = std::get<5>(node);
        bool split_node=false;
        // first, each thread block counts the number of nodes that it needs to

        if (item_ctl.get_local_id(2) == 0) *block_nodes_to_allocate = 0;
        item_ctl.barrier();
    }
}
```

After migration with basic options of DPCT

Question: how can I pass
sycl::nd_item from oneDPL e.g.
std::for_each(policy, iter1, iter2,
SplitNodes())?

--use-experimental-features=free-function-queries

```
struct SplitNodes
{
    int maxPointsPerNode;
    int* node_count;
    int* nodes_allocated;
    int* out_of_space;
    int* child1_;
    int* parent_;
    SplitInfo* splits;

    __device__
    void operator()( thrust::tuple<int&, int&, SplitInfo&, float4&, float4&, int> node )
    {
        int& parent=thrust::get<0>(node);
        int& child1=thrust::get<1>(node);
        SplitInfo& s=thrust::get<2>(node);
        const float4& aabbMin=thrust::get<3>(node);
        const float4& aabbMax=thrust::get<4>(node);
        int my_index = thrust::get<5>(node);
        bool split_node=false;
        // first, each thread block counts the number of nodes that it needs to allocate
        __shared__ int block_nodes_to_allocate;
        if( threadIdx.x== 0 ) block_nodes_to_allocate=0;
        __syncthreads();
```

```
void operator()(std::tuple<int &, int &, SplitInfo &, sycl::float4 &, sycl::float4 &, int> node,
                int *block_nodes_to_allocate, int *block_left, bool *enough_space)
{
    auto item_ctl = sycl::ext::oneapi::experimental::this_nd_item<0>();
    int &parent = std::get<0>(node);
    int &child1 = std::get<1>(node);
    SplitInfo &s = std::get<2>(node);
    const sycl::float4 &aabbMin = std::get<3>(node);
    const sycl::float4 &aabbMax = std::get<4>(node);
    int my_index = std::get<5>(node);
    bool split_node=false;

    if (item_ctl.get_local_id(0) == 0) *block_nodes_to_allocate = 0;
    item_ctl.barrier();
```

Code snippet from - https://github.com/flann-lib/flann/blob/master/src/cpp/flann/algorithms/kdtree_cuda_builder.h

Workarounds

MACRO

- In some complex MACRO cases, DPCT may not be able to correctly deduce the original source line of MACRO
- Simplify complex MACROs in original CUDA code, if migration errors found related to this.

Clang differences

- nvcc-specific behaviors – This issue will be fixed in next release.
[Rodinia] particlefilter - spaces in the triple brackets of kernel invoking e.g. "<<` `< and >>` `>"

Warp with mask not supported by DPCT

```
/*
DPCT1086:0: Migration of __activemask is not supported. You may need to use 0xffffffff instead or
adjust the code.
*/
int __all_sync(unsigned mask, int predicate);
int __any_sync(unsigned mask, int predicate);
unsigned __ballot_sync(unsigned mask, int predicate);
unsigned __activemask();
```

```
214
215     jforce.x = WARP_SHUFFLE(WARP_FULL_MASK, jforce.x, (threadIdx.x+1)&(WARPSIZE-1), WARPSIZE);
216     jforce.y = WARP_SHUFFLE(WARP_FULL_MASK, jforce.y, (threadIdx.x+1)&(WARPSIZE-1), WARPSIZE);
217     jforce.z = WARP_SHUFFLE(WARP_FULL_MASK, jforce.z, (threadIdx.x+1)&(WARPSIZE-1), WARPSIZE);
218     if (doSlow) {
219         jforceSlow.x = WARP_SHUFFLE(WARP_FULL_MASK, jforceSlow.x, (threadIdx.x+1)&(WARPSIZE-1), WARPSIZE);
220         jforceSlow.y = WARP_SHUFFLE(WARP_FULL_MASK, jforceSlow.y, (threadIdx.x+1)&(WARPSIZE-1), WARPSIZE);
221         jforceSlow.z = WARP_SHUFFLE(WARP_FULL_MASK, jforceSlow.z, (threadIdx.x+1)&(WARPSIZE-1), WARPSIZE);
222     }
```

[NAMD] WARP_SHUFFLE with WARP_FULL_MASK could be migrated by DPCT
https://www.ks.uiuc.edu/Research/namd/doxygen/CudaComputeNonbondedKernel_8cu.html

Build script in python

- Intercept-build doesn't support custom build scripts
- Modify python script to dump the commands used for CUDA code build to get a simple Makefile
- Then use intercept-build

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